Optical conductivity and the sum rule in the DDW state

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Abstract

The density-wave with $d-$wave order parameter (DDW) is possibly realized in the underdoped regime of high-T_c cuprates. The DDW state is characterized by two branches of low-lying electronic excitations, and the quantum mechanical current has in particular an inter-branch contribution. The latter component causes a finite-frequency response in the optical conductivity and a reduction of the Drude contribution. We show that this redistribution of the spectral weight leaves the optical sum mostly intact, so that the restricted optical sum rule is only weakly violated.

Key words:
density waves, optical conductivity, optical sum rule

Recently, the interest in charge density waves with unconventional order parameters has increased [1,2,3]. In particular, it has been shown that a charge density wave with d-wave symmetry (DDW) represents a stable state of the $t-J$ model in the large-N limit in certain doping and temperature regions[2]. It thus may be intimately related to the pseudogap phase of high-T$_c$ superconductors[2,3]. The presence of a DDW state should also cause changes in transport coefficients[4]. In the previous paper [6] we showed that the usual expression for the Hall conductivity is modified in the DDW state, due to specific matrix element for the current operator. In the present paper we show that this interband current is responsible for the optical response at higher energies and the reduction of the Drude contribution.

The mean-field Hamiltonian in the DDW state is

$$H = \sum_{\mathbf{k},\sigma} \left[\xi_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + i\Delta_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k+Q},\sigma} + h.c. \right] \qquad (1)$$

Considering nearest and next-nearest neighbor hoppings t and t' and putting the lattice constant of the square lattice to unity, the electronic dispersion is $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu$; we use the abbreviations $\xi_\pm = (\xi_{\mathbf{k}} \pm \xi_{\mathbf{k+Q}})/2$ below. The DDW order parameter is of the form $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y) = -\Delta_{\mathbf{k+Q}}$; here $\mathbf{Q} = (\pi, \pi)$.

The Hamiltonian (1) can be diagonalized [6] by a unitary transformation U so that $\hat{h} \equiv U\hat{H}U^\dagger$ is diagonal and the new quasiparticle energies are

$$\varepsilon_{1,2} = \xi_+ \pm \left[\xi_-^2 + \Delta_{\mathbf{k}}^2 \right]^{1/2} . \qquad (2)$$

The current operator in the DDW state is defined by differentiating $\partial H/\partial k_\alpha = \partial(U^\dagger \hat{h} U)/\partial k_\alpha$. In the new quasiparticle basis it has the components

$$v^\alpha_{1(2)} = \frac{\partial \varepsilon_{1(2)}}{\partial k_\alpha}, \quad v^\alpha_3 = \frac{\xi_-^2}{(\xi_-^2 + \Delta_{\mathbf{k}}^2)^{1/2}} \frac{\partial}{\partial k_\alpha} \frac{\Delta_{\mathbf{k}}}{\xi_-}. \qquad (3)$$

Here the velocities $v_{1(2)}$ correspond to the intraband current operator in the corresponding subband, $\varepsilon_{1(2)}$. The off-diagonal current v_3 arises from the $\mathbf{k}$-dependence of the unitary transformation U, and is the matrix element of the total current operator connecting the two subbands ε_1 and ε_2. It corresponds to the interband transition operator Ω in the notation of

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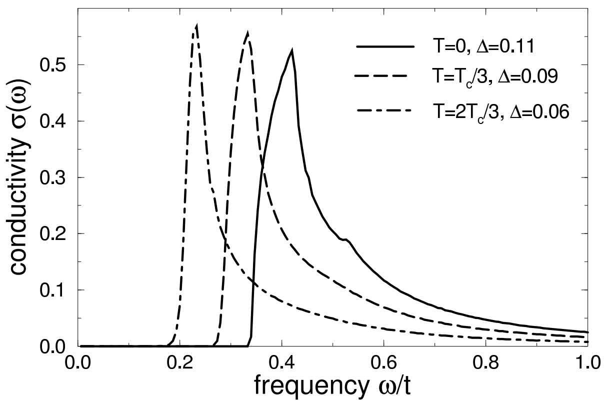

Fig. 1. The evolution of the shape of the optical response below the DDW transition. The $\delta-$function-like Drude peak is not shown here.

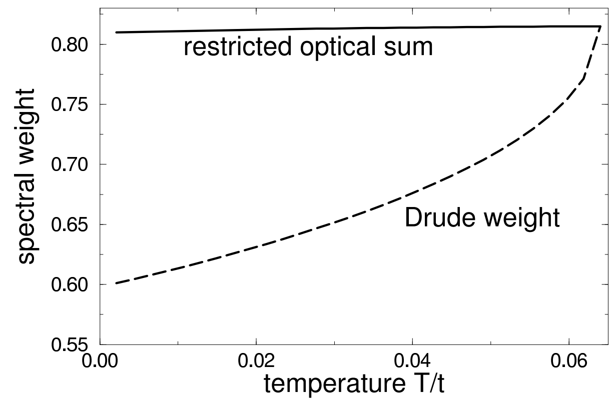

Fig. 2. The temperature dependence of the optical sum and the Drude weight below the DDW transition at $T_c \sim 0.064t$

[5] and is needed for a proper description of the optical response.

The frequency-dependent conductivity has the form $\sigma_\alpha(\omega) = \sigma_\alpha^{(D)}(\omega) + \sigma_\alpha^{(opt)}(\omega)$, where

$$\sigma_\alpha^{(D)} = \frac{e^2\tau}{1+\omega^2\tau^2}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\left[(v_1^\alpha)^2(-\frac{\partial n(\varepsilon_1)}{\partial \varepsilon_1}) + (1\leftrightarrow 2)\right],$$

is the Drude part of $\sigma_\alpha(\omega)$, written for a model with point-like impurities, and

$$\sigma_\alpha^{(opt)} = \frac{\pi e^2}{\omega}\int \frac{d^3\mathbf{k}}{(2\pi)^3}[n(\varepsilon_1) - n(\varepsilon_2)](v_3^\alpha)^2\delta(\omega + \varepsilon_1 - \varepsilon_2) + (1\leftrightarrow 2) \quad (4)$$

is the optical conductivity. Here τ stands for the (large) scattering time, $n(x) = (e^{x/T}+1)^{-1}$.

In rough agreement with [2], we modelled the gap by $\Delta_0 = \bar{\Delta}(T)\sqrt(1+\mu)\Theta(1+\mu)$, where μ is the chemical potential, $\bar{\Delta}(0) = 0.29t$, a BCS temperature dependence is assumed for $\bar{\Delta}(T)$, and t is used as the energy unit. We show the results for the optical conductivity $\sigma_x^{(opt)}$ in Fig. (1) for $t' = 0.3$, $\mu = -0.85$ (doping $\delta \simeq 0.08$), $T_c = 0.064$ and various temperatures.

First, the optical response is non-zero only above the threshold energy $2\Delta_{hs}$, with Δ_{hs} being the value of the gap at the so-called "hot-spots" in $\mathbf{k}-$space where $\xi_\mathbf{k} \simeq \xi_{\mathbf{k}+\mathbf{Q}} \simeq 0$. One has roughly $2\Delta_{hs} \sim 4\Delta_0$ for the above parameters. Beyond its maximum at $\omega \sim 4\Delta_0$, one observes the decay $\sigma_x^{(opt)} \propto \omega^{-3}$ up to energies of the order of the bandwidth. The weight associated with $\sigma_x^{(opt)}$ is $\sim |\Delta_0|/t$ as is suggested by the analysis below.

The restricted optical sum is given by the integral $\int d\omega\sigma_x(\omega)$ which can be easily evaluated for the above $\sigma_\alpha^{(D)}$, $\sigma_\alpha^{(opt)}$. It was shown in [6] that this sum should exhibit a deviation $\sim \Delta^2/E_F$ in the DDW state. At the same time the change in the weight of the Drude peak, $\pi\tau^{-1}\sigma_\alpha(\omega=0)$, is a first-order effect in the DDW state, $\delta\sigma_x(\omega=0) \sim \Delta/E_F$. [6] We illustrate these general findings in Fig. (2). It is seen that the restricted optical sum is nearly unchanged by the formation of the DDW gap, but that the Drude weight exhibits a significant variation below T_c.

Our results for the optical sum differ from those in [7], because there a different spectrum with $t' = 0$ and a much larger value of $\Delta_0(T=0) \sim t$ were used.

In summary, we have shown that the DDW state leads to a shift of the optical spectral weight to higher energies $\sim 4\Delta_0$, but to no change in the optical sum rule in leading order.

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